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Influence of the a-Si:H interfacial region defects on the quasi-static capacitance of Metal/c-Si/SiO_2/a-Si:H structures

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Metal/crystalline silicon/silicon dioxide/hydrogenated amorphous silicon structures (M/c-Si/SiO_2/a-Si:H) are fabricated by thermal oxidation of n^+ doped crystalline Si followed by PECVD deposition of an a-Si:H film. The quasi-static capacitance-voltage (qs C-V) dependencies of the structures are measured using a modification of the standard qs C-V method, which allows reduction of the influence of a-Si:H transient currents. It is shown that the change in the qs C-V curve of the sample caused by thermal annealing with an applied bias can be explained using the defect-pool model for the defects in the a-Si:H. Therefore, the information obtained by qs C-V measurements can be used to characterize the defects close to the insulator/semiconductor interface in PECVD hydrogenated amorphous silicon.

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1. Introduction

Hydrogenated amorphous silicon (a-Si:H) is a material widely used in semiconductor devices, i.e. thin film transistors and solar cells. The quasi-static C-V method applied to Metal-Insulator-Semiconductor (MIS) structures, in which the dielectric layer is SiO_2 or Si_3N_4 and the semiconductor layer is a-Si:H, has been used to study the defects in the gap of amorphous silicon [1,2]. The Metal/c-Si/SiO_2/a-SiGe:H structure has also been used in qs C-V measurements, to determine the defects in the upper part of the gap of hydrogenated a-SiGe [3].

The main difficulties in applying the qs C-V method to MIS structures with hydrogenated amorphous silicon arise from the large transient currents that flow through the semiconductor, especially in the case of undoped layers, and also from the contribution of the interface states to the quasi-static capacitance.

In this work, we show that the main contribution to the qs capacitance of a M/c-Si/SiO_2/a-Si:H structure is due to defects in the a-Si:H interfacial region, and not at the SiO_2/a-Si:H interface. In the measurements, we use a modification of the standard qs C-V method, which allows us to reduce the influence of the transient currents.

2. Experimental details

The experimental structures used in this study were fabricated by thermal oxidation of n^+ doped crystalline Si with a resistivity in the range 0.006-0.015 Ω cm, followed by PECVD deposition of the a-Si:H film. The thickness of the thermal SiO_2 was 140 nm. Undoped a-Si:H with a thickness of about 380 nm was deposited using 10% SiH_4 diluted in H_2 under the following conditions: a frequency of 13.56 MHz, a gas pressure of 0.7 mbar, an applied power of 4 W and a substrate temperature of 200 ^oC. Al metallization of the a-Si:H was carried out through a mask, and capacitors with a diameter of 1 mm were formed. The a-Si:H outside the metal electrode was etched to avoid lateral leakage currents. Al was also used as a back contact to the crystalline silicon. Fig. 1 shows schematically a cross-section of the M/a-Si:H/SiO_2/c-Si structure.

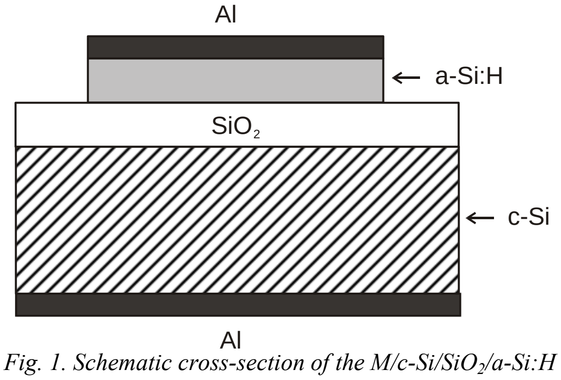

Fig. 1. Schematic cross-section of the M/c-Si/SiO_2/a-Si:H structure.

3. Results and discussion

Fig. 2 shows the influence on the shape and position of the quasi-static C-V curve of thermal annealing and applied bias. The quasi-static C-V curves, normalized to the capacitance of the insulating layer C_I, measured after thermal annealing of the sample at 200 ^oC for 20 min, are shown for three cases: without a bias voltage applied to the control gate (curve 1) and with positive (curves 2, 3) or negative (curves 4, 5) applied bias relative to the top electrode, during the annealing.

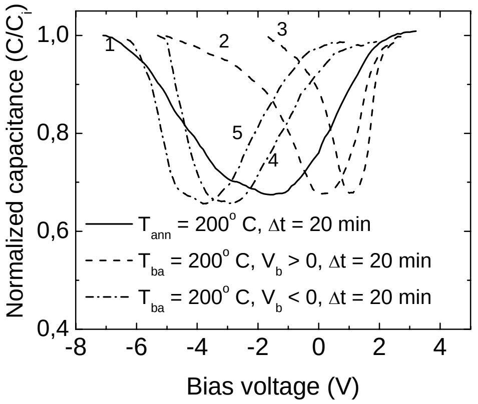

Fig. 2. Experimentally measured qs C-V dependencies obtained after thermal annealing of a structure at 200 ^oC for 20 min and: without applied bias (curve 1), with positive bias - V_{ba} *= 2 V (curve 2) and* V_{ba} *= 3 V (curve 3) and with negative bias -* V_{ba} *= -1V (curve 4) and* V_{ba} *= -2V (curve 5).*

It is seen that bias annealing leads to a narrowing of the qs C-V dependence and to a shift of the curve's minimum to more positive/negative voltages in case of positive/negative applied bias.

Such changes can be explained using the defect-pool model [4]. Indeed, the application of a bias voltage V_b will shift the positions of the conduction and valence bands relative to the Fermi level in the amorphous silicon. According to the defect-pool model, at equilibration temperatures, this will lead to redistribution of the defects in the a-Si:H band gap.

In order to study the influence of the Fermi level position during thermal annealing on the shape of the qs C-V curve, we calculated the C-V dependencies of a M/a-Si:H/SiO$_2$/c-Si structure for two different positions of the Fermi level relative to the conduction band, $E_C - E_F$ = 0.65 eV and 0.85 eV.

The qs C-V curves were calculated [5] as the variation of the total charge ΔQ_T caused by a small change ΔV_G in the applied bias voltage V_G $C(V_G) = \Delta Q_T / \Delta V_G$. The ΔQ_T dependence on ΔV_G was obtained after solving Poisson's equation:

$$\frac{\partial}{\partial x}\left(\varepsilon(x)\frac{\partial}{\partial x}\psi(x)\right) = -\rho(x) \tag{1}$$

numerically in one dimension, using the finite difference method in the whole M/a-Si:H/SiO$_2$/c-Si structure. Here ψ is the potential, ε is the dielectric permittivity and ρ is the charge density. The charge density in the a-Si:H layer has three components, due to free carriers, and those trapped in band tails and deep states. For the valence and conduction band tail distributions, we used exponential dependencies. The dangling bond (DB) contribution to ρ was calculated using the defect-pool expression given in [4]:

$$D(E) = \gamma\left[\frac{2}{f^0(E)}\right]^{\beta kT/E_{v0}} P\left(E + \frac{\beta\sigma^2}{E_{v0}}\right) \tag{2}$$

where *D(E)* is the density of DB states,

$$\gamma = \left[\frac{N_{v0}2E_{v0}^2}{2E_{v0} - kT}\right]^{\beta} H^{1-\beta}\exp\left[-\frac{\beta}{E_{v0}}\left(E_p - E_v - \frac{\beta\sigma^2}{2E_{v0}}\right)\right] \tag{3}$$

$$f^0(E) = \frac{2\exp\left(\frac{E_F - E}{kT}\right)}{1 + 2\exp\left(\frac{E_F - E}{kT}\right) + \exp\left(\frac{2E_F - 2E - U}{kT}\right)} \tag{4}$$

$$P(E) = \frac{1}{\sigma\sqrt{2\pi}}\exp\left[\frac{-(E - E_p)^2}{2\sigma^2}\right] \tag{5}$$

and $\beta = E_{v0}/(E_{v0} + kT)$. In Eqs. (2)-(5), E_{v0} is the characteristic decay energy of the valence band tail, N_{v0} is the density of states at the valence band edge, H is the hydrogen concentration, P(E) is the energy distribution of the sites which would form defects at energy E (the defect-pool function), E_F is the Fermi level, k is the Boltzmann constant, T is the temperature and U is the correlation energy of the amphoteric dangling bond states. P(E) is assumed to be a Gaussian distribution, centered at E_p and having a characteristic width σ. For the one-electron density of states (DOS) due to dangling bonds, we used the approximation [4]:

$$g(E) \approx D(E + kT\ln(2)) + D(E - U - kT\ln(2)) \tag{6}$$

Fig. 3 shows the one-electron density of states in the a-Si:H layer, calculated for the two positions of the Fermi level $E_c - E_F$ = 0.65 eV and $E_c - E_F$ = 0.85 eV, while Figure 4 shows the calculated normalized qs C-V dependencies corresponding to these DOS distributions.

In the calculations, the following parameters were taken as fixed: the characteristic decay energies of the valence and conduction band tails E_{v0} = 0.035 eV, E_{c0} = 0.03 eV, the a-Si:H band gap E_G = 1.75 eV, the position, with respect to the VB edge, of the defect-pool function $E_p - E_v$ = 1.3 eV, the characteristic width of the defect-pool function $\sigma = 0.17$, the correlation energy U = 0.2 eV and the hydrogen concentration H = 5×10^{21} cm^{-3}. It is seen that the shift of the Fermi level from 0.65 eV to 0.85 eV below the conduction band edge changes the one-electron density of states, leading to an increase in the concentration of the D_h states formed as positively charged defects at equilibration and to a decrease in the concentrations of the D_z and D_e states formed as neutral and negatively charged defects.

The qs C-V dependencies shown in Fig. 4 are for a structure with 140 nm thick SiO_2 and 400 nm thick a-Si:H. It is seen that the calculated curve corresponding to the Fermi level lying in the amorphous silicon at 0.85 eV below the conduction band has a sharper minimum, located at a more negative voltage compared to the curve corresponding to E_c - E_F = 0.65 eV. This result is in qualitative agreement with the experimentally measured results, since the application of V_b = -1 V will shift the valence and conductance bands in the a-Si:H in the region close to the a-Si:H/SiO_2 interface upwards, thus increasing the distance between the conduction band edge and the Fermi level.

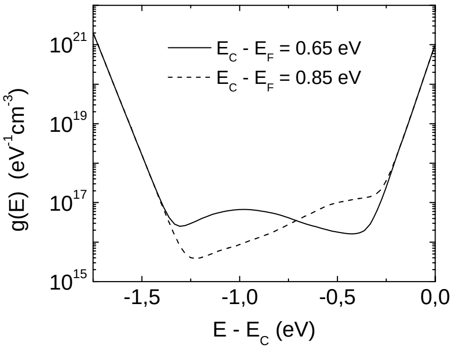

Fig. 3. One electron density of states in the a-Si:H layer calculated at two positions of the Fermi level: $E_C – E_F$ = 0.65 eV (solid line) and $E_C – E_F$ = 0.85 eV (dashed line).

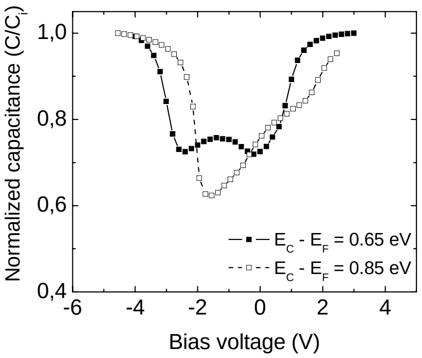

Fig. 4. Calculated normalized qs C-V dependencies corresponding to the one-electron density of states shown in Fig. 3.

Although we made a lot of calculations varying the defect-pool and the hydrogenated amorphous silicon parameters, we were not able to reach a quantitative agreement between the experimental and simulated qs C-V curves. This can be explained in the following way: in the simulations we consider the semiconductor as homogeneously doped, having a fixed distance between the Fermi level and the conduction band edge while in the experiments, during the bias annealing, this distance varies due to band bending in a-Si:H. An additional reason could be the contribution of the states at the a-Si:H/SiO_2 interface, which is not taken in account in our simulations. Nevertheless, the experimental qs C-V dependencies measured after bias annealing show qualitatively the same behavior as the calculated once, i.e. narrowing of the curves and shift of the capacitance minimum, in agreement with the redistribution of defects according to the defect-pool model.

4. Conclusions

Annealing at the equilibration temperature with applied bias of a M/c-Si/SiO_2/a-Si:H structure leads to changes of the shape of the qs C-V curve and the position of its minimum, which are in qualitative agreement with the defect-pool model. Therefore, the information obtained by qs C-V measurements can be used to characterize the defects in the interfacial region of the hydrogenated amorphous silicon close to its interface with the insulator.

Acknowledgements

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